# Geometry of PT-symmetric quantum mechanics

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Recently, much research has been carried out on Hamiltonians that are not Hermitian but are symmetric under space-time reflection, that is, Hamiltonians that exhibit $\mathcal{PT}$ symmetry. Investigations of the Sturm-Liouville eigenvalue problem associated with such Hamiltonians have shown that in many cases the entire energy spectrum is real and positive and that the eigenfunctions form an orthogonal and complete basis. Furthermore, the quantum theories determined by such Hamiltonians have been shown to be consistent in the sense that the probabilities are positive and the dynamical trajectories are unitary. However, the geometrical structures that underlie quantum theories formulated in terms of such Hamiltonians have hitherto not been fully understood. This paper studies in detail the geometric properties of a Hilbert space endowed with a parity structure and analyses the characteristics of a $\mathcal{PT}$-symmetric Hamiltonian and its eigenstates. A canonical relationship between a $\mathcal{PT}$-symmetric operator and a Hermitian operator is established. It is shown that the quadratic form corresponding to the parity operator, in particular, gives rise to a natural partition of the Hilbert space into two halves corresponding to states having positive and negative $\mathcal{PT}$ norm. The indefiniteness of the norm can be circumvented by introducing a symmetry operator $\mathcal{C}$ that defines a positive definite inner product by means of a $\mathcal{CPT}$ conjugation operation.

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## I. INTRODUCTION

In standard quantum mechanics it is assumed that the Hamiltonian $H$ is Hermitian. This requirement ensures that the spectrum of $H$ is real. However, in the past decade many researchers have investigated the consequences of replacing the mathematical requirement of Hermiticity by a more directly physical discrete space-time reflection symmetry known as $\mathcal{PT}$ invariance, where $\mathcal{P}$ is the parity reflection operator and $\mathcal{T}$ is the time reversal operator (Znojil 2004, 2005, 2006, Bender 2005, Geyer *et al.* 2006, Bender 2007). In particular, if $\mathcal{PT}$ symmetry is not broken, that is, if the eigenfunctions of the Hamiltonian $H$ are simultaneously eigenfunctions of the $\mathcal{PT}$ operator, then the spectrum of the Hamiltonian is entirely real (Bender & Boettcher 1998, Bender *et al.* 1999, Dorey *et al.* 2001a, 2001b,

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2007). Furthermore, if a Hilbert space is constructed in terms of an appropriate inner product, then a quantum theory described by a $\mathcal{PT}$-symmetric Hamiltonian exhibits all the desired physical features (Bender *et al.* 2002b, Mostafazadeh 2002).

Hermiticity is a strong condition. Not only does it guarantee the reality of the spectrum, it also generates unitary time evolution. In addition, Hermiticity ties in with a positive definite inner product, which leads to the usual probabilistic interpretation of quantum mechanics. These three results follow naturally from the assumption of Hermiticity. The condition of $\mathcal{PT}$ symmetry is a distinct requirement from Hermiticity. Nevertheless, given the observation that $\mathcal{PT}$-symmetric operators may possess real eigenvalues, it is legitimate to ask (a) whether a physically viable quantum theory can be formulated when we replace the Hermiticity condition with the requirement of space-time reflection symmetry, and (b) whether this new formulation may lead to new physical predictions. Indeed, investigations over the past nine years have shown that by introducing a new symmetry operator denoted as $\mathcal{C}$, a Hilbert space with a positive-definite inner product can be constructed upon which $\mathcal{PT}$-symmetric Hamiltonians act as self-adjoint operators. As a consequence, consistent quantum theories can be formulated via Hamiltonians that possess space-time reflection symmetry but are not Hermitian in the conventional sense.

While many examples of $\mathcal{PT}$-symmetric quantum theories have been analysed in the literature, some of the basic mathematical structures of the theory, such as the geometry of the underlying real Hilbert space in which $\mathcal{PT}$-symmetric quantum theories are defined, have not been fully characterised. The present paper addresses this question by clarifying various mathematical structures of the underlying Hilbert space. For the purpose of constructing a viable quantum theory, we need to consider a framework sufficiently general to admit both the standard theory with a Hermitian Hamiltonian as well as extensions of the standard theory. Thus, we discuss in Section II and Section III the geometrical structures of the underlying real Hilbert space and the role of the observables in conventional quantum mechanics.

In Section IV and Section V we compare the structures described in Sections II and III with the corresponding structures in the quantum theory symmetric under space-time reflection. It is known that the requirement of $\mathcal{PT}$ symmetry alone on the Hamiltonian leads to a state space with an indefinite metric. The important observation we make is that the parity operator associated with space reflection plays the role of an indefinite metric, while the complex structure $J$ of standard quantum mechanics is unaltered in the $\mathcal{PT}$-symmetric theory. This is an attractive feature of $\mathcal{PT}$-symmetric quantum theory from the point of view of complex analysis. We show in Proposition 1 that the squared $\mathcal{PT}$ norm of a state is expressible as a difference of the squared standard Dirac norms of the positive and negative parity parts of the state. Section V also discusses observables. See Mostafazadeh & Batal (2004), Mostafazadeh (2005), and Jones (2005) for previous work on observables in $\mathcal{PT}$-symmetric quantum theories.

In Section VI we analyse the properties of Hamiltonian operators that are symmetric under space-time reflection. It is shown in Proposition 2 that any such Hamiltonian is necessarily expressed as a product of the parity structure and a Hermitian quadratic form. This leads to an alternative way of understanding the reality of the spectrum of such Hamiltonians, as established in Proposition 3, showing that the energy eigenvalues are necessarily real if the corresponding eigenvectors have nonvanishing $\mathcal{PT}$ norms. It is known in the literature that the eigenvalues of $\mathcal{PT}$-symmetric Hamiltonians occur either as real numbers or as complex conjugate pairs. This is shown in Proposition 4. A sufficient condition for the

orthogonality of the eigenstates is then established in Proposition 5. In Section VII we define in geometrical terms a reflection operator $\mathcal{C}$ whose mathematical structure resembles that of a charge operator. This symmetry operator allows us to construct an alternative inner product on the vector space spanned by the eigenfunctions of the $\mathcal{PT}$-symmetric Hamiltonian in terms of $\mathcal{CPT}$-conjugation, thus eliminating states having negative norms. As a consequence, a consistent probabilistic interpretation can be assigned to quantum theories described by $\mathcal{PT}$-symmetric Hamiltonians. To construct the operator $\mathcal{C}$ we establish in Proposition 6 that the eigenfunction associated with a real eigenvalue of a $\mathcal{PT}$-symmetric Hamiltonian is either real or purely imaginary, depending on its parity type. To illustrate these ideas a system of $\mathcal{PT}$-symmetric spin-$\frac{1}{2}$ particles is presented in Section VIII.

## II.   HERMITIAN QUANTUM MECHANICS

Our ultimate objective is to determine the geometric structure of $\mathcal{PT}$-symmetric quantum theory. With this in mind we show in this section how to formulate the geometric structure of standard quantum mechanics. In Sections IV and V we clarify the similarities and differences between the two formalisms. In standard quantum theory Hermitian operators have a dual role as physical observables and as the generators of the dynamics. To understand the relation between these roles it is useful to present quantum mechanics in terms of a primitive underlying even-dimensional *real* Hilbert space $\mathcal{H}$ rather than the complex Hilbert space with respect to which it is usually formulated. We will see that by introducing certain structures on $\mathcal{H}$ we arrive at standard quantum theory. Then by considering an alternative set of structures on $\mathcal{H}$ we arrive at $\mathcal{PT}$-symmetric quantum theory, and the relationship between the two theories becomes clear from a geometric perspective.

Using a standard index notation (see, for example, Geroch 1971, Gibbons & Pohle 1993, Brody & Hughston 1998, 1999 and references cited therein) we let the real vector $\xi^a$ denote a typical element of $\mathcal{H}$. The real Hilbert space $\mathcal{H}$ is to be regarded as coming equipped with a positive definite quadratic form $g_{ab}$ satisfying $g_{ab} = g_{ba}$, with respect to which the squared norm of the vector $\xi^a$ is given by $g_{ab}\xi^a\xi^b$. Then if $\xi^a$ and $\eta^a$ are a pair of elements of $\mathcal{H}$, we define their inner product by $g_{ab}\xi^a\eta^b$.

One can only recover the familiar apparatus of standard quantum mechanics if we further require that $\mathcal{H}$ also be endowed with a compatible complex structure. By a *complex structure* we mean a real tensor $J^a{}_b$ satisfying the following condition:

$$J^a{}_c J^c{}_b = -\delta^a{}_b. \tag{1}$$

The complex structure is then said to be *compatible* with the symmetric quadratic form if $g_{ab}$ and $J^a{}_b$ commute; that is,

$$g_{ab} J^a{}_c J^b{}_d = g_{cd}. \tag{2}$$

If this condition holds, then $g_{ab}$ is said to be *J-invariant*. The compatibility condition is crucial in the case of relativistic fields, where we insist that the creation and annihilation operators satisfy canonical commutation relations (Ashtekar & Magnon 1975).

A straightforward calculation shows that the $J$-invariance of $g_{ab}$ implies that the tensor $\Omega_{ab}$ defined by

$$\Omega_{ab} = g_{ac} J^c{}_b \tag{3}$$

is antisymmetric and nondegenerate, and thus defines a *symplectic structure* on $\mathcal{H}$. To see the antisymmetry of $\Omega_{ab}$, we insert (2) into (3) to obtain $\Omega_{ba} = g_{bc}J^c{}_a = g_{de}J^d{}_b J^e{}_c J^c{}_a = -g_{de}J^d{}_b \delta^e{}_a = -\Omega_{ab}$. The nondegeneracy of $\Omega_{ab}$ becomes clear if we observe that the tensor

$$\Omega^{ab} = g^{ac}g^{cd}\Omega_{cd} \tag{4}$$

acts as the required inverse. Indeed, we have

$$\begin{aligned}
\Omega^{ac}\Omega_{bc} &= g^{ae}g^{cf}g_{eh}J^h{}_f g_{bd}J^d{}_c \\
&= g_{bd}J^d{}_c J^a{}_f g^{cf} \\
&= \delta^a{}_b, \tag{5}
\end{aligned}$$

where in the last step we have used $J$-invariance $J^a{}_c J^b{}_d g^{cd} = g^{ab}$ of the tensor $g^{ab}$. The symplectic structure is also compatible with $J^a{}_b$ in the sense that

$$\Omega_{ab}J^a{}_c J^b{}_d = \Omega_{cd}. \tag{6}$$

This follows because $\Omega_{ab}J^a{}_c J^b{}_d = g_{ae}J^e{}_b J^a{}_c J^b{}_d = -g_{ae}\delta^e{}_d J^a{}_c = -\Omega_{dc} = \Omega_{cd}$. We refer to relation (6) by saying that $\Omega_{ab}$ is $J$-invariant.

With this material at hand we can now elucidate the structure of standard quantum mechanics in geometrical terms. The idea is to endow the real Hilbert space $\mathcal{H}$ with a *Hermitian inner product*. If $\xi^a$ and $\eta^a$ are real Hilbert space vectors, then their Hermitian inner product, which we write as $\langle \eta | \xi \rangle$ using the Dirac notation, is given by the complex expression

$$\langle \eta | \xi \rangle = \tfrac{1}{2}\eta^a(g_{ab} - \mathrm{i}\Omega_{ab})\xi^b. \tag{7}$$

Because the symplectic form $\Omega_{ab}$ is antisymmetric, it follows that, apart from a factor of two, the Hermitian norm agrees with the real Hilbertian norm:

$$\langle \xi | \xi \rangle = \tfrac{1}{2}g_{ab}\xi^a\xi^b. \tag{8}$$

To develop the theory further, we need to complexify the Hilbert space $\mathcal{H}$, and we denote this complexified space by $\mathcal{H}_{\mathbb{C}}$. The elements of $\mathcal{H}_{\mathbb{C}}$ are complex vectors of the form $\xi^a + \mathrm{i}\eta^b$, where $\xi^a$ and $\eta^b$ are elements of the underlying real Hilbert space $\mathcal{H}$.

With the aid of the complex structure, a real Hilbert space vector $\xi^a$ can be decomposed into complex $J$-positive and $J$-negative parts as follows:

$$\xi^a = \xi^a_+ + \xi^a_-, \tag{9}$$

where

$$\xi^a_+ = \tfrac{1}{2}(\xi^a - \mathrm{i}J^a{}_b\xi^b) \quad \text{and} \quad \xi^a_- = \tfrac{1}{2}(\xi^a + \mathrm{i}J^a{}_b\xi^b). \tag{10}$$

For example, in the case of relativistic fields, where $\xi^a$ corresponds to a square-integrable solution of the Klein-Gordon equation defined on a background space-time, this decomposition corresponds to splitting the fields into positive and negative frequency parts. Note that $\xi^a_+$ and $\xi^a_-$ are complex eigenstates of the $J^a{}_b$ operator:

$$J^a{}_b\xi^b_+ = +\mathrm{i}\xi^a_+ \quad \text{and} \quad J^a{}_b\xi^b_- = -\mathrm{i}\xi^a_-. \tag{11}$$

As a consequence, the Hermitian condition (2) implies that two vectors of the same type (for example, a pair of $J$-positive vectors) are necessarily orthogonal with respect to the metric $g_{ab}$. Thus, we have $g_{ab}\xi_+^a \eta_+^b = 0$ for any pair $\xi_+^a$, $\eta_+^a$ of $J$-positive vectors, and $g_{ab}\xi_-^a \eta_-^b = 0$ for any pair $\xi_-^a$, $\eta_-^a$ of $J$-negative vectors.

In the case of a real vector $\xi^a$ it follows from the decomposition (9) that $\xi_-^a = \overline{\xi_+^a}$. We can also split a complex vector into $J$-positive and $J$-negative parts. However, in the case of the splitting of a complex vector $\zeta^a = \zeta_+^a + \zeta_-^a$ there is no *a priori* relationship between the components $\zeta_+^a$ and $\zeta_-^a$. That is, if $\zeta^a$ is not real, then $\zeta_-^a \neq \overline{\zeta_+^a}$. We note that the complex conjugate of a $J$-positive vector is nevertheless a $J$-negative vector, and vice versa. More precisely, we have $\overline{\zeta_+^a} = \bar{\zeta}_-^a$.

In terms of $J$-positive and $J$-negative vectors, the Dirac inner product (7) takes a simplified form:

$$\langle \eta | \xi \rangle = \eta_-^a g_{ab} \xi_+^b. \tag{12}$$

Equations (7) and (12) are equivalent as we verify below:

$$\begin{aligned}
\eta_-^a g_{ab} \xi_+^b &= \tfrac{1}{4}(\eta^a + \mathrm{i}J^a{}_c \eta^c)g_{ab}(\xi^b - \mathrm{i}J^b{}_d \xi^d) \\
&= \tfrac{1}{4}\left(g_{ab} + J^c{}_a J^d{}_b g_{cd}\right)\eta^a \xi^b - \tfrac{1}{4}\mathrm{i}\left(g_{ac}J^c{}_b - J^c{}_a g_{bc}\right)\eta^a \xi^b \\
&= \tfrac{1}{2}\eta^a(g_{ab} - \mathrm{i}\Omega_{ab})\xi^b.
\end{aligned} \tag{13}$$

Here we have used the relation (2) and the antisymmetry of $\Omega_{ab}$.

## III.  QUANTUM-MECHANICAL OBSERVABLES

In this section we show how to represent the observables of standard quantum mechanics in terms of the geometry of the real Hilbert space $\mathcal{H}$. A quantum-mechanical observable corresponds to a real symmetric $J$-invariant quadratic form on $\mathcal{H}$, that is, to a real tensor $F_{ab}$ satisfying the symmetry condition

$$F_{ab} = F_{ba} \tag{14}$$

and the $J$-invariance condition

$$F_{ab}J^a{}_c J^b{}_d = F_{cd}. \tag{15}$$

Note in particular that the quadratic form $g_{ab}$ satisfies (14) and (15); $g_{ab}$ is the observable corresponding to the identity. For the expectation value of the observable $F$ in the state $\xi^a$ we have

$$\frac{\langle \xi | F | \xi \rangle}{\langle \xi | \xi \rangle} = \frac{F_{ab}\xi^a \xi^b}{g_{ab}\xi^a \xi^b}, \tag{16}$$

and more generally given the states $\xi^a$ and $\eta^a$ we have

$$\langle \eta | F | \xi \rangle = \eta_-^a F_{ab} \xi_+^b. \tag{17}$$

The quantum *operator* associated with the observable $F_{ab}$ is obtained by raising one of the indices with the inverse of the metric:

$$F^a{}_b = g^{ac} F_{cb}. \tag{18}$$

Then, since $F_{ab}$ is $J$-invariant, it follows that when the quantum operator $F^a{}_b$ acts on a $J$-positive state vector, the result is another $J$-positive state vector. Alternative ways of writing (17) are

$$\langle \eta | F | \xi \rangle = \eta^a_- g_{ac} F^c{}_b \xi^b_+ = F^a{}_c \eta^c_- g_{ab} \xi^b_+, \tag{19}$$

which express the self-adjointness of $F^a{}_b$ with respect to the Dirac Hermitian inner product.

Let us consider now the symmetries of the Hilbert space $\mathcal{H}$. The rotations of $\mathcal{H}$ around the origin are represented as orthogonal transformations, which are matrix operations of the form $\xi^a \to M^a{}_b \xi^b$ such that

$$g_{ab} M^a{}_c M^b{}_d = g_{cd}. \tag{20}$$

Such transformations preserve the norm $g_{ab} \xi^a \xi^b$ of the state $\xi^a$. The unitary group then consists of orthogonal matrices that also leave the symplectic structure invariant:

$$\Omega_{ab} M^a{}_c M^b{}_d = \Omega_{cd}. \tag{21}$$

In the case of an infinitesimal orthogonal transformation of the form

$$M^a{}_b = \delta^a{}_b + \epsilon f^a{}_b \tag{22}$$

with $\epsilon^2 \ll 1$, it is straightforward to verify that $f^a{}_b$ satisfies

$$g_{ac} f^c{}_b + g_{bc} f^c{}_a = 0, \tag{23}$$

from which we deduce that $f^a{}_b$ has the form

$$f^a{}_b = g^{ac} f_{cb}, \tag{24}$$

where $f_{ab}$ is antisymmetric. Substituting (24) into (22) and then into (21) shows that for $M^a{}_b$ to be a unitary operator it is necessary and sufficient that $f_{ab}$ be $J$-invariant. This shows that any infinitesimal unitary transformation can be written in the form

$$M^a{}_b = \delta^a{}_b + \epsilon J^a{}_c F^c{}_b, \tag{25}$$

where $F^a{}_b$ is the operator associated with the quantum observable $F_{ab}$. Conversely, $f_{ab}$ is antisymmetric and $J$-invariant if and only if it can be expressed in the form

$$f_{ab} = F_{ac} J^c{}_b, \tag{26}$$

where $F_{ab}$ is symmetric and $J$-invariant. Note that if $F^a{}_b$ is proportional to the identity $g^a{}_b$, then (25) corresponds to an infinitesimal phase transformation. Also, if $F^a{}_b$ is trace-free, then (25) gives rise to an infinitesimal special unitary transformation.

Thus, the *operator* $F^a{}_b$ is associated with both the observable $F_{ab}$ as well as the infinitesimal unitary transformation

$$\xi^a \to \xi^a + \epsilon J^a{}_b F^b{}_c \xi^c. \tag{27}$$

The complete trajectory of the unitary transformation associated with the operator $F^a{}_b$ can be obtained by exponentiating (27) and writing

$$\xi^a(t) = \exp\left( t J^b{}_c F^c{}_d \xi^d \partial_b \right) \xi^a \Big|_{\xi^a = \xi^a(0)}, \tag{28}$$

where $\partial_b = \partial/\partial\xi^b$. The differential operator in the exponent can be written as

$$J^b{}_c F^c{}_d \xi^d \partial_b = \tfrac{1}{2} \left( \Omega^{ab} \partial_b F \right) \partial_a, \tag{29}$$

where $F(\xi) = F_{ab}\xi^a\xi^b$. Thus, we see that the quadratic form $F_{ab}\xi^a\xi^b$ is the generator of a Hamiltonian vector field $X^a(\xi) = \partial\xi^a/\partial t$ on $\mathcal{H}$ given by

$$\frac{\partial\xi^a}{\partial t} = \tfrac{1}{2}\Omega^{ab}\partial_b F(\xi). \tag{30}$$

In other words, the trajectory of the one-parameter family of unitary transformations associated with the observable $F_{ab}$ is generated by the Hamiltonian vector field $\tfrac{1}{2}\Omega^{ab}\partial_b F(\xi)$. If $H(\xi) = H_{ab}\xi^a\xi^b$ denotes the quadratic function on $\mathcal{H}$ associated with the Hamiltonian of a standard quantum system, then the Schrödinger equation can be written in the form

$$\frac{\partial\xi^a}{\partial t} = \tfrac{1}{2}\Omega^{ab}\partial_b H. \tag{31}$$

We have shown how to describe standard quantum mechanics in terms of the geometry of a real vector space $\mathcal{H}$ equipped with a complex structure $J^a{}_b$, a positive-definite quadratic form $g_{ab}$, and a compatible symplectic structure $\Omega_{ab}$. Observables are represented by $J$-invariant quadratic forms on $\mathcal{H}$ and dynamical trajectories are given by the symplectic vector field on $\mathcal{H}$ generated by such forms. These structures are intrinsic to standard quantum theory.

## IV.   SPACE-TIME REFLECTION SYMMETRY

In Section III we showed that to describe standard quantum theory geometrically it is necessary to introduce a complex structure tensor $J^a{}_b$ on the underlying space $\mathcal{H}$ of real state vectors. The remaining structures, namely, the positive definite quadratic form $g_{ab}$ and the symplectic structure $\Omega_{ab}$, are then chosen to satisfy the compatibility conditions. In this section we show how to represent geometrically a $\mathcal{PT}$-symmetric quantum theory. To do so, we will replace the metric $g_{ab}$ of standard quantum mechanics by a new quadratic form $\pi_{ab}$ called *parity*. The novelty of this approach is that unlike $g_{ab}$, the quadratic form $\pi_{ab}$ is not positive definite. We will see that the parity operator can only be introduced if the dimension of the complex vector space of $J$-positive vectors is even.

Recall that in standard quantum mechanics the parity operator $\pi^a{}_b$ represents space reflection and therefore it satisfies the conditions of an observable, as discussed in the previous section. This means that $\pi_{ab} = g_{ac}\pi^c{}_b$ is required to be real and symmetric. In addition it must satisfy the $J$-invariance condition

$$\pi_{ab}J^a{}_c J^b{}_d = \pi_{cd}, \tag{32}$$

which is equivalent to the commutation relation

$$\pi^a{}_c J^c{}_b = J^a{}_c \pi^c{}_b. \tag{33}$$

In addition, the parity operator is required to satisfy the orthogonality condition

$$g_{ab}\pi^a{}_c \pi^c{}_b = g_{cd}. \tag{34}$$

As a consequence, the eigenvalues of the parity operator are $\pm 1$, as we now show: Since $\pi_{ab}$ is symmetric, the orthogonality condition (34) reads

$$\pi^a{}_c \pi^c{}_b = \delta^a{}_b. \tag{35}$$

Thus, repeated space reflection is equivalent to the identity. If we diagonalise $\pi^a{}_b$, the diagonal entries must be $\pm 1$. Once the number of positive and negative eigenvalues is known, then the parity operator is unique up to unitary transformations. To see this, suppose that $\mathcal{P}$ and $\mathcal{P}'$ are distinct parity operators. Because they have the same spectrum, there exists a unitary transformation that maps one into the other.

In this paper we make the further assumption that the parity operator is trace-free:

$$\pi^a{}_a = 0. \tag{36}$$

This condition may not be essential (see Bender *et al.* 2002a), but for simplicity we insist that the condition (36) be satisfied so that half of the eigenvalues are $+1$ and the other half of the eigenvalues are $-1$. As a consequence, $\pi^a{}_b$ defines a special unitary operator on the space of $J$-positive vectors associated with $\mathcal{H}$. The trace-free condition also implies that the parity operator can only be defined if the dimension of the underlying real Hilbert space $\mathcal{H}$ is a multiple of four.

To formulate a $\mathcal{PT}$-symmetric quantum theory, we keep the real Hilbert space $\mathcal{H}$ with its complex structure $J^a{}_b$, and introduce a new inner product on $\mathcal{H}$ that is defined in terms of the parity operator. In particular, we introduce a $\mathcal{PT}$ inner product $\langle \eta \| \xi \rangle$ for the pair of elements $\xi^a$ and $\eta^a$ in $\mathcal{H}$ according to

$$\langle \eta \| \xi \rangle = \tfrac{1}{2} \eta^a (\pi_{ab} - \mathrm{i}\omega_{ab}) \xi^b, \tag{37}$$

where $\omega_{ab}$ is defined by

$$\omega_{ab} = \Omega_{ac} \pi^c{}_b. \tag{38}$$

Equivalently, from (3) we have

$$\omega_{ab} = \pi_{ac} J^c{}_b. \tag{39}$$

Since $\pi_{ab}$ is an observable in standard quantum mechanics, it follows that $\omega_{ab}$ is antisymmetric and thus defines a new symplectic structure on $\mathcal{H}$ that is compatible with the complex structure $J^a{}_b$. Indeed, one can easily verify the $J$-invariance condition

$$\omega_{ab} J^a{}_c J^b{}_d = \omega_{cd} \tag{40}$$

associated with the symplectic structure $\omega_{ab}$. We remark that a Hilbert space endowed with the inner product (37) is known as the Pontrjagin space (Pontrjagin 1944), the properties of which have been investigated by Kreĭn and collaborators (Kreĭn 1965, Azizov 1994). For recent work on the relation between the Kreĭn space and $\mathcal{PT}$ symmetry, see Langer & Tretter (2004), Güenther *et al.* (2005), Tanaka (2006), and Mostafazadeh (2006).

As in standard quantum mechanics, the $\mathcal{PT}$ inner product (37) can be written directly in terms of the $J$-positive and $J$-negative parts of the vectors $\xi^a$ and $\eta^a$. Recall in this connection that splitting $\mathcal{H}$ into $J$-positive and $J$-negative parts only depends on the complex structure $J^a{}_b$, and not on the associated quadratic forms. A short calculation shows that

$$\langle \eta \| \xi \rangle = \eta^a_- \pi_{ab} \xi^b_+. \tag{41}$$

Conversely, from (41) we get

$$\eta^a_- \pi_{ab} \xi^b_+ = \tfrac{1}{4}(\eta^a + \mathrm{i}J^a{}_c \eta^c)\pi_{ab}(\xi^b - \mathrm{i}J^b{}_d \xi^d) \tag{42}$$

by virtue of (10). Then, using the $J$-invariance of $\pi_{ab}$ and the antisymmetry of $\omega_{ab}$, as defined by (38), we are immediately led back to the inner product (37).

We now demonstrate the $\mathcal{P}$-invariance of $\omega_{ab}$. We begin by raising the indices of the quadratic form $\pi_{ab}$ using the metric $g^{ab}$:

$$\pi^{ab} = g^{ac}g^{bd}\pi_{cd}. \tag{43}$$

We then multiply $\pi^{bc}$ by $\pi_{ab}$. Using (35) we find that

$$\pi_{ab}\pi^{bc} = \delta_a{}^c. \tag{44}$$

Thus $\pi^{ab}$, as defined in (43), is the inverse of $\pi_{ab}$. It is straightforward to verify that the analogously defined tensor

$$\omega^{ab} = g^{ac}g^{bd}\omega_{cd} \tag{45}$$

satisfies

$$\omega^{ab} = \pi^{ac}\pi^{bd}\omega_{cd} \tag{46}$$

and

$$\omega_{ab}\omega^{bc} = \delta_a{}^c. \tag{47}$$

Equation (47) shows that $\omega^{ab}$ is the inverse of $\omega_{ab}$. Also, from (45) and (46) we deduce that

$$\pi_a{}^c\pi_b{}^d\omega_{cd} = \omega_{ab}, \tag{48}$$

which shows that $\omega_{ab}$ is $\mathcal{P}$-invariant.

We summarise these results by observing that for the Hermitian theory we have the compatible system of structures $(J^a{}_b, g_{ab}, \Omega_{ab})$ on $\mathcal{H}$, whereas the quantum theory symmetric under space-time reflection comes equipped with the compatible system of structures $(J^a{}_b, \pi_{ab}, \omega_{ab})$. The key difference between the two theories is that while $g_{ab}$ is positive definite, $\pi_{ab}$ is indefinite with the split signature $(+, \cdots, +, -, \cdots, -)$. In particular, given a state $\xi^a$, its $\mathcal{PT}$ norm, or more precisely its pseudo-norm, is defined by the expression

$$\langle \xi \| \xi \rangle = \tfrac{1}{2}\pi_{ab}\xi^a \xi^b. \tag{49}$$

This norm can be either positive or negative and in some cases may even vanish.

To interpret the $\mathcal{PT}$ norm we establish some identities concerning the parity splitting of the Hilbert space. Given any real element $\xi^a$ in $\mathcal{H}$, we can split it into its positive and negative parity parts by writing

$$\xi^a = \xi^a_\oplus + \xi^a_\ominus, \tag{50}$$

where

$$\xi^a_\oplus = \tfrac{1}{2}(\xi^a + \pi^a{}_b \xi^b) \quad \text{and} \quad \xi^a_\ominus = \tfrac{1}{2}(\xi^a - \pi^a{}_b \xi^b). \tag{51}$$

These vectors are eigenstates of the parity operator $\pi_{ab}$, satisfying

$$\pi^a{}_b \xi^b_\oplus = \xi^a_\oplus \quad \text{and} \quad \pi^a{}_b \xi^b_\ominus = -\xi^a_\ominus. \tag{52}$$

If we write

$$\Pi^a_{\oplus b} = \tfrac{1}{2}(\delta^a{}_b + \pi^a{}_b) \quad \text{and} \quad \Pi^a_{\ominus b} = \tfrac{1}{2}(\delta^a{}_b - \pi^a{}_b) \tag{53}$$

for the projection operators onto positive and negative parity eigenstates, then we have

$$\delta^a{}_b = \Pi^a_{\oplus b} + \Pi^a_{\ominus b} \quad \text{and} \quad \pi^a{}_b = \Pi^a_{\oplus b} - \Pi^a_{\ominus b}, \tag{54}$$

where

$$\Pi^a_{\oplus b} \xi^b = \xi^a_\oplus \quad \text{and} \quad \Pi^a_{\ominus b} \xi^b = \xi^a_\ominus. \tag{55}$$

Because $\pi^a{}_b$ and $J^a{}_b$ commute, it follows that the positive parity component of the $J$-positive part of a real vector $\xi^a$ agrees with the $J$-positive part of the positive parity part of $\xi^a$, and likewise for other such combinations. This observation allows us to establish the following result for the $\mathcal{PT}$ norm:

**Proposition 1** *The squared $\mathcal{PT}$ norm of a state $\xi^a \in \mathcal{H}$ is given by the difference between the squared Hermitian norm of the positive parity part $\xi^a_\oplus$ of the state and the squared Hermitian norm of the negative parity part $\xi^a_\ominus$ of the state:*

$$\langle \xi \| \xi \rangle = \langle \xi_\oplus | \xi_\oplus \rangle - \langle \xi_\ominus | \xi_\ominus \rangle. \tag{56}$$

It follows from this proposition that if a measurement of the parity of a state is more likely to yield a positive result, then its $\mathcal{PT}$ norm is positive. Conversely, for a state having more probably negative parity, its $\mathcal{PT}$ norm is negative. To prove the identity (56) we insert (54) into (49) and use the relations (55) for the parity eigenstates.

We observe finally that if $\xi^a$ and $\eta^a$ are positive and negative parity states, respectively, then their standard quantum transition amplitude vanishes:

$$\langle \xi_\oplus | \eta_\ominus \rangle = 0. \tag{57}$$

We derive (57) from (7) by substituting $\eta^a_\ominus$ for $\eta^a$ and $\xi^a_\oplus$ for $\xi^a$ and then using the identities

$$g_{ab} \Pi^a_{\oplus c} \Pi^b_{\ominus d} = 0 \quad \text{and} \quad \Omega_{ab} \Pi^a_{\oplus c} \Pi^b_{\ominus d} = 0. \tag{58}$$

The second of these two relations follows from the first because the $J$-tensor commutes with the parity projection operators.

## V.  OBSERVABLES AND SYMMETRIES

In this section we examine the transformations of $\mathcal{H}$ that preserve the $\mathcal{PT}$ norm $\pi_{ab}\xi^a\xi^b$. Any linear transformation has the general form $\xi^a \to M^a{}_b\xi^b$, and this transformation preserves the $\mathcal{PT}$ norm for all $\xi^a \in \mathcal{H}$ if and only if

$$\pi_{ab}M^a{}_c M^b{}_d \xi^c\xi^d = \pi_{ab}\xi^a\xi^b \tag{59}$$

for all $\xi^a$. For an infinitesimal transformation

$$M^a{}_b = \delta^a{}_b + \epsilon f^a{}_c, \tag{60}$$

(59) holds to first order in $\epsilon$ if and only if

$$\pi_{ab}f^a{}_c \xi^b\xi^c = 0 \tag{61}$$

for all $\xi^a$. We deduce that $f^a{}_b$ must have the form

$$f^a{}_b = \pi^{ac} f_{cb}, \tag{62}$$

where $f_{bc}$ is antisymmetric. Here, as in the previous section, $\pi^{ab}$ denotes the inverse of $\pi_{ab}$ and satisfies $\pi^{ab}\pi_{bc} = \delta^a{}_c$, and we note that $\pi^{ab}$ can be defined unambiguously in this way without reference to $g_{ab}$.

To verify (62) we observe that if (61) holds for all $\xi^a$, then $\pi_{ab}f^b{}_c$ must be antisymmetric. Writing $\pi_{ab}f^b{}_c = f_{ac}$, we then obtain (62) by applying the inverse of $\pi_{ab}$ to each side of the equation. Thus, the infinitesimal pseudo-orthogonal transformations that preserve the $\mathcal{PT}$ norm are given by

$$M^a{}_b = \delta^a{}_b + \epsilon\pi^{ac} f_{cb}, \tag{63}$$

where $f_{ab}$ is antisymmetric.

Next we require that the transformations preserve the $\mathcal{PT}$ symplectic structure $\omega_{ab}$. By virtue of the compatibility condition, this is equivalent to the condition that the complex structure is preserved. To first order in $\epsilon$ we have

$$\omega_{ab}M^a{}_c M^b{}_d = \omega_{cd} + \epsilon\left(\omega_{ad}\pi^{ae} f_{ec} + \omega_{cb}\pi^{be} f_{ed}\right). \tag{64}$$

Thus, for $\omega_{ab}$ to be preserved we require that

$$\omega_{ad}\pi^{ae} f_{ec} + \omega_{cb}\pi^{be} f_{ed} = 0. \tag{65}$$

However, since $\omega_{ab} = \pi_{ac}J^c{}_b$, the condition (65) implies that $f_{ab}$ is $J$-invariant. Because $f_{ab}$ is antisymmetric and $J$-invariant, it can be written in the form

$$f_{ab} = F_{ac}J^c{}_b, \tag{66}$$

where $F_{ab}$ is a $J$-invariant symmetric quadratic form on $\mathcal{H}$.

We conclude that the general infinitesimal pseudo-unitary transformation preserving $\pi_{ab}$ and $\omega_{ab}$ has the form

$$M^a{}_b = \delta^a{}_b + \epsilon\omega^{ac} F_{cb}, \tag{67}$$

where $F_{ab}$ is a standard quantum observable in the sense that it is symmetric and $J$-invariant. It is interesting to recall equation (26) and to note that the same $J$-invariant quadratic forms on $\mathcal{H}$ appear in standard quantum theory as well as in $\mathcal{PT}$ symmetric quantum theory.

Following the approach of Section III, we can express the trajectory of the pseudo-unitary transformation associated with the operator $F^a{}_b = \pi^{ac} F_{cb}$ in the form

$$\xi^a(t) = \exp\left(t\omega^{bc} F_{cd}\xi^d\partial_b\right)\xi^a\Big|_{\xi^a=\xi^a(0)}, \tag{68}$$

where $\partial_b = \partial/\partial\xi^b$. Therefore, if we write $F(\xi) = F_{ab}\xi^a\xi^b$ for the quadratic function on $\mathcal{H}$ associated with a given observable $F_{ab}$, then the dynamical equation for the corresponding one-parameter family of pseudo-unitary transformations on $\mathcal{H}$ preserves the $\mathcal{PT}$ inner product, and this equation can be expressed in Hamiltonian form as

$$\frac{\partial\xi^a}{\partial t} = \tfrac{1}{2}\omega^{ab}\partial_b F. \tag{69}$$

This result is analogous to (31) for the case of standard quantum mechanics.

## VI. $\mathcal{PT}$-SYMMETRIC HAMILTONIAN OPERATORS

In this section we consider observables that are invariant under space-time reflection symmetry. Specifically, we consider the properties of $\mathcal{PT}$-symmetric Hamiltonian operators. In contrast to the Hermiticity condition in conventional quantum mechanics, here we demand that the Hamiltonian be invariant under space-time reflection. In ordinary quantum mechanics the Hermiticity condition on the Hamiltonian operator is that $H^a{}_b$ be real,

$$H^a{}_b = \bar{H}^a{}_b, \tag{70}$$

and $J$-invariant,

$$J^a{}_b H^b{}_c J^c{}_d = H^a{}_d. \tag{71}$$

If a Hamiltonian operator satisfies these conditions, then we say it is Hermitian. In our discussion of $\mathcal{PT}$-symmetric Hamiltonian operators, we shall keep the $J$-invariance, but replace the reality condition by one that has a nice physical interpretation, namely, invariance under space-time reflection.

In the previous sections we introduced the real vector space $\mathcal{H}$ and the complex structure $J^a{}_b$ on it. Then we showed that this structure can be augmented in one of two ways, either by introducing the positive definite symmetric quadratic form $g_{ab}$ and the associated symplectic structure $\Omega_{ab}$, or by introducing the split-signature indefinite form $\pi_{ab}$ and the associated symplectic structure $\omega_{ab}$. In the following, we will consider either the structure $(J^a{}_b, g_{ab}, \Omega_{ab})$ or the structure $(J^a{}_b, \pi_{ab}, \omega_{ab})$, or sometimes both. For simplicity of terminology we call the former the $g$-structure on $\mathcal{H}$ and the latter the $\pi$-structure on $\mathcal{H}$.

We begin by considering those aspects of the $\mathcal{PT}$-symmetric theory that arise when we have only the $\pi$-structure on $\mathcal{H}$ at our disposal, and we will make no direct use of the parity operator $\pi^a{}_b = g^{ac}\pi_{cb}$ because this involves $g_{ab}$. We make the following definitions: Suppose that $\mathcal{H}$ is endowed with a $\pi$-structure and let $H^a{}_b$ be a complex operator on $\mathcal{H}_{\mathbb{C}}$ so that $H^a{}_b = X^a{}_b + iY^a{}_b$, where $X^a{}_b$ and $Y^a{}_b$ are real. Assume that $H^a{}_b$ is $J$-invariant. Then $H^a{}_b$

is said to be *invariant under space-time reflection*, or $\mathcal{PT}$ symmetric, with respect to the given $\pi$-structure if

$$\pi_{bc}\bar{H}^c{}_d\pi^{ad} = H^a{}_b. \tag{72}$$

This relation states that if we take the complex conjugate of the Hamiltonian followed by a parity transformation, we recover the original Hamiltonian.

Now we discuss the important notion of a Hermitian form. A tensor $K_{ab}$ on $\mathcal{H}_{\mathbb{C}}$ is said to be a *Hermitian form* if it is $J$-invariant and satisfies

$$\bar{K}_{ab} = K_{ba}. \tag{73}$$

Thus, $K_{ab}$ is a Hermitian form if $K_{ab} = X_{ab}+\mathrm{i}Y_{ab}$, where $X_{ab}$ and $Y_{ab}$ are real and $J$-invariant, and $X_{ab}$ is symmetric and $Y_{ab}$ is antisymmetric. In particular, $g_{ab} - \mathrm{i}\Omega_{ab}$ and $\pi_{ab} - \mathrm{i}\omega_{ab}$ are examples of Hermitian forms. The following proposition is a direct consequence of these definitions:

**Proposition 2** *A Hamiltonian operator $H^a{}_b$ is $\mathcal{PT}$ symmetric with respect to the $\pi$-structure $(J^a{}_b, \pi_{ab}, \omega_{ab})$ if and only if there exists a Hermitian form $K_{ab}$ such that*

$$H^a{}_b = \pi^{ac}K_{bc}. \tag{74}$$

Proposition 2 demonstrates that the condition of $\mathcal{PT}$ symmetry on a Hamiltonian is a kind of Hermiticity condition, albeit not the conventional one. It is possible to characterise $\mathcal{PT}$ invariance completely without involving any elements of the $g$-structure on $\mathcal{H}$. To verify (74) we note that

$$\pi_{bc}\bar{H}^c{}_d\pi^{ad} = \pi_{bc}\pi^{ce}\bar{K}_{de}\pi^{ad} = \delta_b{}^e K_{ed}\pi^{ad} = H^a{}_b. \tag{75}$$

Let us turn now to the analysis of the spectrum of the operator $H^a{}_b$, still keeping within the context of the $\pi$-structure. Because $H^a{}_b$ is complex, we have to admit the possibility of complex eigenvectors, that is, elements of $\mathcal{H}_{\mathbb{C}}$. The following definition simplifies the exposition: If $\phi^a$ is an element of $\mathcal{H}_{\mathbb{C}}$, then we define its $\mathcal{PT}$ norm by the expression $\pi_{ab}\phi^a\bar{\phi}^b$, which is the sum of the $\mathcal{PT}$ norms of the real and imaginary parts of $\phi^a$.

**Proposition 3** *If the $\mathcal{PT}$ norm of an eigenvector of a $\mathcal{PT}$-symmetric Hamiltonian is non-vanishing, then the corresponding eigenvalue is real.*

*Proof.* Suppose that for some possibly complex value of $E$ the vector $\phi^a$, which may also be complex, satisfies the eigenvalue equation $H^a{}_b\phi^b = E\phi^a$. The complex conjugate of this equation is $\bar{H}^a{}_b\bar{\phi}^b = \bar{E}\bar{\phi}^a$. Transvecting each side of these equations with $\pi_{ca}$, we then obtain

$$\pi_{ca}H^a{}_b\phi^b = E\pi_{ca}\phi^a \quad \text{and} \quad \pi_{ca}\bar{H}^a{}_b\bar{\phi}^b = \bar{E}\pi_{ca}\bar{\phi}^a. \tag{76}$$

Therefore, by Proposition 2 we deduce that

$$K_{ab}\phi^b = E\pi_{ab}\phi^b \tag{77}$$

and that

$$\bar{K}_{ab}\bar{\phi}^b = \bar{E}\pi_{ab}\bar{\phi}^b. \tag{78}$$

Because $K_{ab}$ is a Hermitian form, we can replace (78) with the relation

$$K_{ab}\bar{\phi}^b = \bar{E}\pi_{ab}\bar{\phi}^b. \tag{79}$$

If we contract (77) and (79) with $\bar{\phi}^a$ and $\phi^a$, respectively, and subtract, we obtain

$$(E - \bar{E})\pi_{ab}\phi^a\bar{\phi}^b = 0, \tag{80}$$

which establishes Proposition 3. $\qquad\square$

We conclude that if a $\mathcal{PT}$-symmetric Hamiltonian has complex eigenvalues, then the corresponding eigenstates necessarily have a vanishing $\mathcal{PT}$ norm. We proceed to augment the vector space $\mathcal{H}$ with the $g$-structure as well as the $\pi$-structure. Introducing the $g$-structure allows us to consider the parity operator $\pi^a_{\ b}$. The condition (72) for the invariance under space-time reflection can now be written in the form

$$\pi^a_{\ c}\bar{H}^c_{\ d}\pi^d_{\ b} = H^a_{\ b}. \tag{81}$$

Another way of stating this condition is that the real part of the Hamiltonian operator has even parity and the imaginary part of the Hamiltonian has odd parity. Therefore, if we write $H^a_{\ b} = X^a_{\ b} + iY^a_{\ b}$, where $X^a_{\ b}$ and $Y^a_{\ b}$ are real, then we have

$$\pi^a_{\ c}X^c_{\ d}\pi^d_{\ b} = X^a_{\ b} \quad \text{and} \quad \pi^a_{\ c}Y^c_{\ d}\pi^d_{\ b} = -Y^a_{\ b}. \tag{82}$$

Conversely, any such complex operator is automatically invariant under space-time reflection.

With the aid of the parity operator $\pi^a_{\ b}$ we are led to the following observation on the reality of the energy eigenvalues:

**Proposition 4** *Let $E$ and $\phi^a$ be an eigenvalue and corresponding eigenstate of a $\mathcal{PT}$-symmetric Hamiltonian operator $H^a_{\ b}$. Then, $\bar{E}$ is also an eigenvalue of $H^a_{\ b}$, for which the associated eigenstate is $\pi^a_{\ b}\bar{\phi}^b$. In particular, if $\phi^a$ is a simultaneous eigenstate of the $\mathcal{PT}$ operator, then $E$ is real.*

*Proof.* We start from the eigenvalue equation

$$H^a_{\ b}\phi^b = E\phi^a, \tag{83}$$

where $E$ may or may not be real. Substituting (81) into the right side of (83) gives

$$\pi^a_{\ c}\bar{H}^c_{\ d}\pi^d_{\ b}\phi^b = E\phi^a. \tag{84}$$

By taking the complex conjugate, we obtain $\pi^a_{\ c}H^c_{\ d}\pi^d_{\ b}\bar{\phi}^b = \bar{E}\bar{\phi}^a$. We then multiply on the left by the parity operator and get

$$H^a_{\ b}\pi^b_{\ c}\bar{\phi}^c = \bar{E}\pi^a_{\ b}\bar{\phi}^b. \tag{85}$$

Thus, if $\phi^a$ is an energy eigenstate with eigenvalue $E$, then the state defined by $\pi^a_{\ b}\bar{\phi}^b$ is another energy eigenstate having eigenvalue $\bar{E}$. If, in addition, the eigenstate $\phi^a$ is simultaneously an eigenstate of the $\mathcal{PT}$ operator, then

$$\pi^a_{\ b}\bar{\phi}^b = \lambda\phi^a, \tag{86}$$

where $\lambda$ is a pure phase. Substituting (86) into (85) and subtracting the result from (83), we get $\bar{E} = E$, which establishes Proposition 4. $\qquad\square$

Dorey *et al.* (2001a,b) showed that the key condition of Proposition 4, namely, that $\phi^a$ is a simultaneous eigenstate of $\mathcal{PT}$, is in fact valid for the Hamiltonian $H = p^2 + x^2(ix)^\epsilon$ ($\epsilon > 0$). When energy eigenstates $\{\phi_n^a\}$ are not simultaneously eigenstates of the $\mathcal{PT}$ operator, we say that space-time reflection symmetry is *broken* (Bender & Boettcher 1998, Bender *et al.* 1999). In this case, the complex eigenvalues $\{E_n\}$ occur in complex conjugate pairs. Conversely, if space-time reflection symmetry is unbroken so that $\{\phi_n^a\}$ are eigenstates of the $\mathcal{PT}$ operator, then the corresponding energy eigenvalues are real. In this case, a sufficient (but not necessary) condition for the orthogonality of the eigenstates can be given:

**Proposition 5** *If the eigenstates $\{\phi_n^a\}$ of a $\mathcal{PT}$-symmetric Hamiltonian operator $H^a_{\ b}$ are simultaneously eigenstates of the $\mathcal{PT}$ operator, then a sufficient condition for the orthogonality of the eigenstates with respect to the $\mathcal{PT}$ inner product is that the quadratic form defined by $H_{ab} = g_{ac}H^c_{\ b}$ is symmetric.*

*Proof.* Consider for $n \neq m$ a pair of eigenvalue equations $H^a_{\ b}\phi_n^b = E_n\phi_n^a$ and $H^a_{\ b}\phi_m^b = E_m\phi_m^a$. Transvecting these equations with $\pi_{ac}\bar{\phi}_m^c$ and $\pi_{ac}\bar{\phi}_n^c$, respectively, and subtracting the two resulting equations, we obtain

$$\bar{\phi}_m^c \pi_{ca} H^a_{\ b}\phi_n^b - \bar{\phi}_n^c \pi_{ca} H^a_{\ b}\phi_m^b = \pi_{ab}\left( E_n\phi_n^b\bar{\phi}_m^a - E_m\phi_m^b\bar{\phi}_n^a \right). \qquad (87)$$

Now, if the energy eigenstates are simultaneously eigenstates of the $\mathcal{PT}$ operator so that $\pi^a_{\ b}\bar{\phi}_n^b = \phi_n^a$, then $\pi_{ab}\bar{\phi}_n^b = g_{ab}\phi_n^b$. Therefore, the left side of (87) becomes

$$\phi_m^c g_{ca} H^a_{\ b}\phi_n^b - \phi_n^c g_{ca} H^a_{\ b}\phi_m^b = H_{cb}\left( \phi_m^c\phi_n^b - \phi_n^c\phi_m^b \right), \qquad (88)$$

where $H_{cb} = g_{ca}H^a_{\ b}$. Therefore, the condition $H_{cb} = H_{bc}$ is sufficient to ensure that the right side of (87) vanishes, which establishes Proposition 5. $\qquad\square$

Note that although the symmetric condition on the complex Hamiltonian $H_{ab}$ is sufficient to ensure the orthogonality of the eigenstates, it is not a necessary condition.

## VII.   CONSTRUCTION OF A POSITIVE INNER PRODUCT

In this section we use an additional symmetry operator $\mathcal{C}$ to construct a positive-definite inner product. It is necessary to do this because when one formulates quantum mechanics on a Hilbert space endowed with the structure of space-time reflection symmetry, one obtains an indefinite metric having a split signature, where half of the quantum states have positive and the other half have negative $\mathcal{PT}$ norm. The split signature arises because half of the eigenvalues of the parity structure $\pi_{ab}$ are positive and the other half are negative.

The norm in standard quantum mechanics is closely related to the probabilistic interpretation of the theory. Therefore, the physical interpretation of the inner product defined in (37) is ambiguous. To remedy this difficulty, Mostafazadeh (2002) and Bender *et al.* (2002b, 2003) pointed out the existence of a new symmetry associated with complex non-Hermitian Hamiltonians that are symmetric under space-time reflection. It was noted that by use of this symmetry, which carries an interpretation similar to that of charge conjugation, it is possible to introduce a new inner product on the vector space $\mathcal{H}_{\mathbb{C}}$ spanned by the eigenstates of $\mathcal{PT}$-symmetric Hamiltonians in such a way that all the eigenstates have positive-definite

norm. With the aid of this symmetry the correct probabilistic interpretation of the quantum theory is restored. Here, we discuss briefly the geometrical properties of the symmetry associated with the new symmetry operator $C^a_{\ b}$. We begin by establishing a formula for the $\mathcal{PT}$ inner product of a pair of energy eigenstates:

**Proposition 6** *Suppose that $H^a_{\ b}$ is a $\mathcal{PT}$-symmetric Hamiltonian operator whose $\mathcal{PT}$ symmetry is not broken so that its energy eigenvalues are real. Let $\{\phi^a_n\}$ denote a set of eigenstates of $H^a_{\ b}$. Then the $\mathcal{PT}$ inner product of an arbitrary pair of energy eigenstates is*

$$\langle \phi_m \| \phi_n \rangle = g_{ab} \phi^a_n \phi^b_m. \tag{89}$$

Recall that the $\mathcal{PT}$ inner product of a pair of states is given by $\pi_{ab} \phi^a_n \bar{\phi}^b_m$. Proposition 4 states that when the $\mathcal{PT}$ symmetry is unbroken, $\phi^a_n$ is an eigenstate of the $\mathcal{PT}$ operator. We thus have $\pi_{ab} \phi^a_n \bar{\phi}^b_m = g_{ac} \pi^c_{\ b} \phi^a_n \bar{\phi}^b_m = g_{ac} \phi^a_n \phi^b_m$, which establishes Proposition 6. Because the $\mathcal{PT}$ norms of the energy eigenstates are real, it follows that the real part of $\phi^a_n$ is orthogonal to its imaginary part with respect to the quadratic form $g_{ab}$.

We normalise the energy eigenstates according to the scheme

$$\phi^a_n \rightarrow \frac{1}{\sqrt{|g_{ab} \phi^a_n \phi^b_n|}} \phi^a_n, \tag{90}$$

and assume hereafter that $\phi^a_n$ will always be normalised in this way. It was shown in Section IV that half of the normalised energy eigenstates have positive $\mathcal{PT}$ norm and that the remaining half have negative $\mathcal{PT}$ norm. Without loss of generality we may order the levels so that

$$g_{ab} \phi^a_m \phi^b_n = (-1)^n \delta_{nm}. \tag{91}$$

With these conventions at hand, we define the new symmetry operator $C^a_{\ b}$. First, $C^a_{\ b}$ is a $\mathcal{PT}$-symmetric operator. This implies that there exists a positive Hermitian form $L_{ab}$ satisfying $\bar{L}_{ab} = L_{ba}$ such that we can write $C^a_{\ b} = \pi^{ac} L_{bc}$. Second, $C^a_{\ b}$ commutes with the Hamiltonian operator $H^a_{\ b}$. As a consequence, the eigenstates $\{\phi^a_n\}$ of the Hamiltonian are simultaneous eigenstates of $C^a_{\ b}$. Third, the eigenvalues of $C^a_{\ b}$ are given by

$$C^a_{\ b} \phi^b_n = (-1)^n \phi^a_n, \tag{92}$$

where $\phi^a_n$ satisfies (91). In other words, $C^a_{\ b}$ is an operator commuting with the Hamiltonian $H^a_{\ b}$ such that its eigenvalues are precisely the $\mathcal{PT}$ norm of the corresponding eigenstates. Consequently, $C^a_{\ b}$ is involutary, satisfying $C^a_{\ b} C^b_{\ c} = \delta^a_{\ c}$, and trace-free so that $C^a_{\ a} = 0$.

We remark that in the infinite-dimensional context, it has been shown that the $\mathcal{C}$ operator admits a position-space representation of the form (Mostafazadeh 2002, Bender *et al.* 2002b)

$$\mathcal{C} = \sum_n \phi_n(x) \phi_n(y), \tag{93}$$

in contrast with the position-space representation for the parity operator

$$\mathcal{P} = \sum_n (-1)^n \phi_n(x) \phi_n(-y). \tag{94}$$

Here $\{\phi_n(x)\}$ denote eigenfunctions of the $\mathcal{PT}$-symmetric Hamiltonian.

Having defined the operator $C^a{}_b$, we introduce on the vector space $\mathcal{H}_{\mathbb{C}}$ the following inner product: If $\xi^a, \eta^a \in \mathcal{H}_{\mathbb{C}}$, then their quantum-mechanical inner product $\langle \xi | \eta \rangle$ is defined by

$$\langle \xi | \eta \rangle = g_{ac} C^c{}_b \pi^b{}_d \eta^a \bar{\xi}^d. \tag{95}$$

With respect to the inner product $\langle \cdot | \cdot \rangle$ we have

$$\langle \phi_n | \phi_m \rangle = g_{ac} C^c{}_b \pi^b{}_d \phi_m^a \bar{\phi}_n^d = g_{ac} C^c{}_b \phi_m^a \phi_n^b = (-1)^n g_{ab} \phi_m^a \phi_n^b = \delta_{nm}. \tag{96}$$

Therefore, (95) defines a positive-definite inner product between elements of $\mathcal{H}_{\mathbb{C}}$. Note that this notation makes no distinction between the Dirac Hermitian inner product defined in (7) and the inner product (95) defined with respect to $\mathcal{CPT}$ conjugation. We view (95) as a natural extension of (7) because when the prescribed Hamiltonian is Hermitian, (95) reduces to the conventional Dirac inner product (7).

## VIII.  AN EXPLICIT TWO-DIMENSIONAL CONSTRUCTION

Consider a quantum-mechanical system of a spin-$\frac{1}{2}$ particle whose Hamiltonian $H$ is a $2 \times 2$ complex matrix. We regard $H$ as an operator that acts on the space of $J$-positive vectors. The general form of the two-dimensional parity operator satisfying the properties described above is $\mathcal{P} = \boldsymbol{\sigma} \cdot \mathbf{n}$, where $\mathbf{n}$ is an arbitrary *real* unit vector and $\boldsymbol{\sigma}$ are the Pauli matrices. However, because in finite dimensions $\mathcal{P}$ is determined uniquely up to unitary transformations, we can set $\mathbf{n} = (1, 0, 0)$, so that the parity operator is given by

$$\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{97}$$

Based on Wigner's discussion on time reversal in quantum mechanics (Wigner 1932), we remark that the corresponding operator is *antiunitary*. We recall in this connection that a unitary operator $T$ in conventional quantum mechanics has the norm-preserving property $\langle \varphi | \psi \rangle = \langle T\varphi | T\psi \rangle$, whereas if $T$ is antiunitary we have a 'transposed' form of the norm-preserving property $\langle \varphi | \psi \rangle = \langle T\psi | T\varphi \rangle$ (Wigner 1960a,b). In particular, for a spin system in Hermitian quantum mechanics the Hamiltonian must be invariant under time reversal (Morpurgo & Touschek 1954).

For the present consideration we let time-reversal acting on a symmetric Hamiltonian be given by complex conjugation. It follows that a Hamiltonian satisfying the condition $\mathcal{P} \bar{H} \mathcal{P} = H$ can be expressed as

$$H = \begin{pmatrix} r \mathrm{e}^{\mathrm{i}\theta} & s \\ s & r \mathrm{e}^{-\mathrm{i}\theta} \end{pmatrix}. \tag{98}$$

This is the example considered by Bender *et al.* (2002b, 2003). [A number of other papers have been written on $\mathcal{PT}$-symmetric matrix Hamiltonians. See, for example, Znojil (2001), Mostafazadeh (2002), Weigert (2006), Güenther *et al.* (2007).] The Hamiltonian (98) can alternatively be expressed in the form

$$H = r \cos \theta \mathbb{1} + \tfrac{1}{2} \omega \, \boldsymbol{\sigma} \cdot \mathbf{n}, \tag{99}$$

where $\omega^2 = s^2 - r^2 \sin^2 \theta$ and $\mathbf{n} = 2\omega^{-1}(s, 0, ir \sin \theta)$ is a *complex* unit vector satisfying $\mathbf{n} \cdot \mathbf{n} = 1$. Therefore, we see that while a Hermitian Hamiltonian for a spin-$\frac{1}{2}$ particle can also be written in the form (99), the key difference here is that the unit vector $\mathbf{n}$ in the case of a $\mathcal{PT}$-symmetric system is, in general, complex. This is the sense in which we are extending quantum mechanics into complex domain.

According to Proposition 2 this operator can be expressed as a product of the quadratic form representing the parity operator and a standard Hermitian quadratic form. Thus, we have

$$\begin{pmatrix} re^{i\theta} & s \\ s & re^{-i\theta} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} s & re^{i\theta} \\ re^{-i\theta} & s \end{pmatrix}. \tag{100}$$

Although $H$ is a complex matrix, the secular equation for the eigenvalues of this Hamiltonian is *real* (Bender *et al.* 2002b). The energy eigenvalues

$$E_\pm = r \cos \theta \pm \sqrt{s^2 - r^2 \sin^2 \theta} \tag{101}$$

are also real and nondegenerate in the parameter region determined by

$$s^2 > r^2 \sin^2 \theta. \tag{102}$$

We demand that this inequality be satisfied so that the $\mathcal{PT}$ symmetry is not broken. If the $\mathcal{PT}$ symmetry is broken, then the energy eigenvalues $E_+$ and $E_-$ are complex, and according to the result of the previous section the $\mathcal{PT}$ norm of the corresponding eigenstates must vanish. To verify that the norm vanishes in this case, we first determine the unnormalised energy eigenstates and obtain the expression

$$|E_\pm\rangle = \begin{pmatrix} 1 \\ -i\frac{r}{s}\sin\theta \pm \sqrt{1 - (\frac{r}{s}\sin\theta)^2} \end{pmatrix}. \tag{103}$$

Now, if the $\mathcal{PT}$ symmetry is broken so that $s^2 < r^2 \sin^2 \theta$, then it follows that the second components of the vectors $|E_\pm\rangle$ are purely imaginary. Recall that if $|v\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ is a two-component vector, then the application of the $\mathcal{PT}$ operation gives $\mathcal{PT}|v\rangle = (\bar{v}_2 \ \ \bar{v}_1)$. Therefore, in the broken symmetry phase, we have

$$\langle E_\pm \| E_\pm \rangle \Big|_{\text{broken } \mathcal{PT}} = 0, \tag{104}$$

as claimed.

We now turn to consider the physically interesting situation where the parameters in the Hamiltonian satisfy (102) so that the $\mathcal{PT}$ symmetry is unbroken. In this case we have the orthogonality condition $\langle E_\pm \| E_\mp \rangle = 0$. The eigenvectors $|E_\pm\rangle$ of the Hamiltonian $H$ are simultaneously eigenstates of the $\mathcal{PT}$ operator. As denoted earlier, we can choose the phases of the eigenvectors so that their eigenvalues under $\mathcal{PT}$ are all unity. For this choice of phases these eigenvectors are given by

$$|E_+\rangle = \frac{1}{\sqrt{2\cos\alpha}} \begin{pmatrix} e^{i\alpha/2} \\ e^{-i\alpha/2} \end{pmatrix}, \quad |E_-\rangle = \frac{i}{\sqrt{2\cos\alpha}} \begin{pmatrix} e^{-i\alpha/2} \\ -e^{i\alpha/2} \end{pmatrix}. \tag{105}$$

Here we have set $\sin\alpha = (r/s)\sin\theta$, and the inequality (102) for the reality of $E_\pm$ ensures that $\alpha$ is real and that both $st$ and $\cos\alpha$ are positive. It is easy to verify that these states are also eigenstates of $\mathcal{PT}$ with unit eigenvalues.

In conventional Hermitian quantum mechanics the norm is defined in terms of a Hermitian inner product, which has the form $\langle u|v \rangle = \bar{u} \cdot v$ and which equals $\bar{u}_1 v_1 + \bar{u}_2 v_2$ in two dimensions. Thus, the norm $\langle v|v \rangle$ of a vector is positive definite. On the other hand, the $\mathcal{PT}$ inner product is determined by the $\mathcal{PT}$ conjugation operation $\langle u\|v \rangle = \mathcal{PT} u \cdot v$, which is $\bar{u}_2 v_1 + \bar{u}_1 v_2$ in two dimensions. Note that $\overline{\mathcal{PT} u \cdot v} = u \cdot \mathcal{PT} v$. Just as in the case of the Hermitian norm, the $\mathcal{PT}$ norm $\langle v\|v \rangle$ is also independent of overall phase. With respect to the $\mathcal{PT}$ inner product there is an indefinite norm given by $\langle E_+\|E_+ \rangle = +1$ and $\langle E_-\|E_- \rangle = -1$, as well as the orthogonality conditions $\langle E_-\|E_+ \rangle = \langle E_+\|E_- \rangle = 0$. These identities can easily be verified by use of (105).

The eigenvectors $|E_\pm \rangle$ are complete in that they span the two dimensional vector space. The statement of completeness is embodied in the identity

$$\|E_+\rangle\langle E_+\| - \|E_-\rangle\langle E_-\| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{106}$$

where $\|v\rangle\langle v\|$ denotes $|v\rangle\langle \mathcal{PT} v|$. Equation (106) is the $\mathcal{PT}$-symmetric version of the statement of completeness $|E_+\rangle\langle E_+| + |E_-\rangle\langle E_-| = \mathbb{1}$ in a Hermitian quantum theory.

The $\mathcal{C}$ operator is given by $\boldsymbol{\sigma} \cdot \mathbf{n}$, or more specifically by:

$$\mathcal{C} = \frac{1}{\cos\alpha} \begin{pmatrix} \mathrm{i}\sin\alpha & 1 \\ 1 & -\mathrm{i}\sin\alpha \end{pmatrix}. \tag{107}$$

Note that $[\mathcal{C}, \mathcal{PT}] = 0$ and $[\mathcal{P}, \mathcal{T}] = 0$ implies $\mathcal{CPT} = \mathcal{TPC}$. Therefore, if $|v\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ is an arbitrary two-component vector, we have

$$\mathcal{CPT}[|v\rangle] = \mathcal{T}\left[\frac{1}{\cos\alpha} \begin{pmatrix} 1 & \mathrm{i}\sin\alpha \\ -\mathrm{i}\sin\alpha & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}\right]$$
$$= \frac{1}{\cos\alpha}\left( \bar{v}_1 + \mathrm{i}\bar{v}_2\sin\alpha \quad \bar{v}_2 - \mathrm{i}\bar{v}_1\sin\alpha \right) = \langle v|. \tag{108}$$

It follows that

$$\langle v|u \rangle = \frac{1}{\cos\alpha} \left( \bar{v}_1 u_1 + \bar{v}_2 u_2 + \mathrm{i}(\bar{v}_2 u_1 - \bar{v}_1 u_2)\sin\alpha \right) \tag{109}$$

for the $\mathcal{CPT}$ inner product of a pair of vectors. In particular, it is straightforward to verify that $\langle E_\pm|E_\mp \rangle = 0$ and that $\langle E_\pm|E_\pm \rangle = 1$. It also follows that the squared $\mathcal{CPT}$ norm of an arbitrary vector $|v\rangle$, given by

$$\langle v|v \rangle = \frac{1}{\cos\alpha} \left( \bar{v}_1 v_1 + \bar{v}_2 v_2 + \mathrm{i}(\bar{v}_2 v_1 - \bar{v}_1 v_2)\sin\alpha \right), \tag{110}$$

is real and positive (because $\bar{v}_2 v_1 - \bar{v}_1 v_2$ is purely imaginary) and that the constraint (102) is satisfied.

We observe that by the introduction of the additional structure $\mathcal{C}$ it is possible to restore a fully consistent quantum theory of a $\mathcal{PT}$-symmetric spin-$\frac{1}{2}$ particle system. It should be noted, however, that the example considered here is by no means the most general form of a complex extension of a two-level system in quantum mechanics, as it is evident from the special form $\mathbf{n} = 2\omega^{-1}(s, 0, \mathrm{i}r\sin\theta)$ of the unit vector used in (99).

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